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Following Osipov and Hiller, a generalized heat kernel expansion is considered for the effective action of bosonic operators. In this generalization, the standard heat kernel expansion, which counts inverse powers of a c-number mass parameter, is extended by allowing the mass to be a matrix in flavor space. We show that the generalized heat kernel coefficients can be related to the standard ones in a simple way. This holds with or without trace and integration over spacetime, to all orders and for general flavor spaces. Gauge invariance is manifest.

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Let the bosonic operator be

$$\Delta = -D^2 + U(x), \quad D_\mu = \partial_\mu + A_\mu(x), \quad (1)$$

where the gauge field $A_\mu(x)$ and the scalar field $U(x)$ are matrices in some flavor space. This kind of operators appear frequently in the computation of the effective action of fermions (see e.g. [1]). In particular the normal parity component of such an effective action is directly related to the determinant of the operator $\Delta = D^\dagger D$ (D being the Dirac operator). A standard technical device to compute the effective action is to split the scalar field into two contributions

$$U(x) = m^2 + Y(x) \quad (2)$$

where m^2 is a constant c-number (squared) mass parameter. This allows to carry out an expansion in inverse powers of m^2 with coefficients which are homogeneous polynomials constructed with the quantities Y and D_μ . These coefficients are ordered by its scale dimension and thus they are identical to those of the standard heat kernel expansion [2–4]. These coefficients are very well-known and we refer to [1,5] for details.

In the context of effective theories of quarks aiming at modeling QCD at low energy [6], Osipov and Hiller [7,8] consider instead a more general separation of the scalar field

$$U(x) = M + Y(x) \quad (3)$$

where M is still a constant (i.e. x -independent) but not necessarily a c-number. In general M is a matrix in flavor

space. In a typical application $M = \text{diag}(m_1^2, \dots, m_n^2)$ for n flavors, m_i being the constituent quark mass of the i -th flavor, and $Y(x)$ accounts for the deviations of the scalar field from M . Obviously in the particular case of degenerated masses the previous case $M = m^2$ (a c-number) is recovered.

One can try to carry out an expansion in inverse powers of M (i.e. a large mass expansion) in this more general setting. A straight approach is to organize the expansion in such a way that each term is again a homogeneous polynomial in D_μ and Y . Technically this can be done by introducing a bookkeeping parameter λ

$$\Delta_\lambda = M - \lambda D^2 + \lambda Y(x), \quad (4)$$

and then proceed to expand the effective action in powers of λ . This simple minded approach, however, meets the problem that gauge invariance is not preserved separately by each term of the expansion [7,8]. (Of course gauge invariance holds for the full effective action functional.) The problem is that we want to regard Δ , as well as its associated effective action, as a functionals where the external fields A_μ and Y are the true variables and M and the operator ∂_μ play the role of fixed parameters, i.e.

$$\Delta = \Delta(A, Y) = M - D^2 + Y(x). \quad (5)$$

From this point of view, under a gauge transformation ($\Omega(x)$ being a matrix in flavor space)

$$\Omega^{-1}(x) \Delta(Y, A) \Omega(x) = \Delta(Y^\Omega, A^\Omega). \quad (6)$$

The quantities M and ∂_μ are gauge invariant by definition, D_μ and U transform homogeneously under a similarity transformation and the external fields A_μ and Y transform inhomogeneously:

$$\begin{aligned} \partial_\mu^\Omega &= \partial_\mu, & M^\Omega &= M \\ D_\mu^\Omega &= \Omega^{-1} D_\mu \Omega, & U^\Omega &= \Omega^{-1} U \Omega \\ A_\mu^\Omega &= A_\mu + \Omega^{-1} [D_\mu, \Omega], & Y^\Omega &= Y + \Omega^{-1} [U, \Omega]. \end{aligned} \quad (7)$$

It is clear now that, because λ does not affect M in Δ_λ , the expansion in λ breaks gauge invariance, i.e. in general $\Delta_\lambda(Y^\Omega, A^\Omega)$ will not coincide with $\Omega^{-1} \Delta_\lambda(Y, A) \Omega$ at $\lambda \neq 1$. They do coincide when $M = m^2$ is a c-number and in this case the standard heat kernel expansion is recovered.

As an aside, we note that manifest gauge invariance is automatic order by order in the context of a strict derivative expansion of the effective action functional (e.g. [9]), that is considering instead $\Delta_\lambda = U(x) - \lambda D^2$. The strict derivative expansion can be viewed as a resummation of the heat kernel expansion to all orders in Y . Recently explicit closed formulas have been obtained in such an expansion for both the normal and the abnormal parity components of the effective action of fermions coupled to vector, axial, scalar and pseudo-scalar external fields and for an arbitrary flavor group [10,11]. In the normal parity case the formulas hold for arbitrary space-time dimension through fourth order in the covariant derivatives. In the abnormal parity case the leading order is computed in two and four dimensions.

The problem of obtaining a manifestly gauge invariant inverse mass expansion for matricial M has been solved by Osipov and Hiller in [7,8] and explicit results are presented there for lowest orders in the case of two and three flavors without gauge fields. Presently we reformulate their approach in a way that makes it simple to treat the case of arbitrary flavor group and the introduction of gauge fields. Finally we find a simple relation between the generalized heat kernel coefficients and the standard ones so that no new calculation of these coefficients from scratch is required.

In order to present the formalism let X and Z denote two matrices (or operators) in some space V , such that the combination $X + Z$ transforms by a similarity transformation, X represents the term which is defined to be invariant under gauge transformations and Z transforms inhomogeneously (thus, X , Z and $X + Z$ generalize M , Y and U respectively). Consider now the *gauge covariant* quantity $f(X + Z)$ where $f(x)$ is some arbitrary function such as e.g. the logarithm. (Note that f itself is a c-number although its argument, and thus its value, can be a matrix.) Loosely speaking what we are seeking is to obtain an expansion for small Z (or large X) that generalizes the usual Taylor expansion valid for c-number X and Z (or more generally, valid when X and Z commute), but in such a way that each term of the expansion is separately gauge covariant. This can be achieved as follows. Let the coefficients Z_n be defined by set of relations

$$(X + Z)^n = \sum_{k=0}^n \binom{n}{k} \langle X^{n-k} \rangle Z_k(Z, X), \quad n = 0, 1, 2, \dots \quad (8)$$

In this formula the notation $\langle A \rangle$ represents an average of a matrix A in V , namely

$$\langle A \rangle = \frac{\text{tr}(A)}{\text{tr}(1)}, \quad (9)$$

where tr denotes the trace operation in V . The coefficients Z_n are matrices and are recursively defined by the

formula. The depend both on Z and X in general. Of course when X is a c-number Z_n is simply Z^n .

Since $\{x^n, n = 0, 1, 2, \dots\}$ is a basis of functions we can take linear combinations in the previous formula and write more generally

$$f(X + Z) = \sum_{n=0}^{\infty} \frac{1}{n!} \langle f^{(n)}(X) \rangle Z_n, \quad (10)$$

where $f(x)$ is an arbitrary function and $f^{(n)}(x)$ is its n -th derivative.¹ Note that the coefficients Z_n do not depend on the function $f(x)$.

Three crucial properties of these coefficients can be established without explicit computation:

(i) The Z_n depend on Z and X but this dependence is such that Z_n remains unchanged if X is replaced by $X + a$ where a is any c-number:

$$Z_n(Z, X) = Z_n(Z, X + a). \quad (11)$$

This is because the shift introduced by a can be absorbed by a redefinition of $f(x)$.

(ii) The coefficients are gauge covariant since $(X + Z)^n$ is covariant and $\langle X^n \rangle$ is invariant for all n :

$$Z_n(Z^\Omega, X) = \Omega^{-1} Z_n(Z, X) \Omega, \quad Z^\Omega = \Omega^{-1}(X + Z)\Omega - X. \quad (12)$$

(iii) For the traced quantity

$$\text{tr} f(X + Z) = \sum_{n=0}^{\infty} \frac{1}{n!} \langle f^{(n)}(X) \rangle z_n, \quad z_n = \text{tr}(Z_n). \quad (13)$$

Then, the z_n vanish for vanishing Z , except z_0 which equals $\text{tr}(1)$.

$$z_n(0, X) = 0 \quad (n > 0). \quad (14)$$

This latter property distinguishes this expansion from other possible expansions which also enjoy the properties (i) and (ii), for instance

$$f(X + Z) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(\langle X \rangle) Z'_n. \quad (15)$$

The correct choice of $\langle f(X) \rangle$ among other possible choices is a merit of [7,8].

At lowest orders

¹As usual in quantum field theory, we will be happy if the formulas hold in the sense of asymptotic series. They are not required nor expected to be convergent.

$$\begin{aligned}
Z_0 &= 1, \\
Z_1 &= Z + \bar{X}, \\
Z_2 &= (Z + \bar{X})^2 - \bar{x}_2, \\
Z_3 &= (Z + \bar{X})^3 - 3\bar{x}_2(Z + \bar{X}) - \bar{x}_3,
\end{aligned} \tag{16}$$

where we have introduced the following notation

$$\bar{X} = X - \langle X \rangle, \quad \bar{x}_n = \langle \bar{X}^n \rangle. \tag{17}$$

For the traced coefficients

$$\begin{aligned}
z_0 &= \text{tr}(1), \\
z_1 &= \text{tr}(Z), \\
z_2 &= \text{tr}(Z^2 + 2\bar{X}Z), \\
z_3 &= \text{tr}(Z^3 + 3\bar{X}Z^2 + 3(\bar{X}^2 - \bar{x}_2)Z).
\end{aligned} \tag{18}$$

The property (i) noted above is manifest since Z_n depends on \bar{X} only (and is independent of $\langle X \rangle$). Gauge covariance is also obvious since Z_n comes as a combination of powers of $Z + \bar{X}$, and this matrix transforms covariantly.

For subsequent application in the effective action problem some properties of the Z_n will be needed. First note that by taking a first order variation with respect to Z , either in (8) or (10), and using the identity

$$\delta \text{tr}(f(X + Z)) = \text{tr}(f'(X + Z)\delta Z), \tag{19}$$

it follows that

$$\frac{\delta z_n}{\delta Z} = nZ_{n-1}, \tag{20}$$

which is well-known in the context of the heat kernel expansion [1]. Next note that from their definition (8) and the property (11) above, which allows to use \bar{X} instead of X , one has to all orders

$$Z_n = (Z + \bar{X})^n - \sum_{k=0}^{n-2} \binom{n}{k} \bar{x}_{n-k} Z_k \tag{21}$$

$$= \sum_{k=0}^n \beta_{n,k} (Z + \bar{X})^k \tag{22}$$

for some c-number coefficients $\beta_{n,k}$. However, use of (20) immediately implies that

$$\beta_{n,k} = \frac{n}{k} \beta_{n-1,k-1} = \dots = \frac{n!}{k!} \beta_{n-k,0} \tag{23}$$

and thus (defining $\beta_n = \beta_{n,0}$)

$$Z_n = \sum_{k=0}^n \frac{n!}{k!} \beta_{n-k} (Z + \bar{X})^k. \tag{24}$$

The recurrence (21) then takes the form

$$\beta_n = \delta_{n,0} - \sum_{k=2}^n \frac{\bar{x}_k}{k!} \beta_{n-k}, \tag{25}$$

and for lowest orders yields

$$\begin{aligned}
\beta_0 &= 1, \\
\beta_1 &= 0, \\
\beta_2 &= -\frac{\bar{x}_2}{2!}, \\
\beta_3 &= -\frac{\bar{x}_3}{3!}, \\
\beta_4 &= -\frac{\bar{x}_4}{4!} + \frac{\bar{x}_2}{4},
\end{aligned} \tag{26}$$

Note that this differs from the usual cumulant expansion beyond third order.

A further identity will be needed to relate the standard and generalized heat kernel coefficients. Let

$$\hat{T}_X = \sum_{r=0}^{\infty} \beta_r \left(\frac{\partial}{\partial \langle X \rangle} \right)^r. \tag{27}$$

Here $\partial/\partial \langle X \rangle$ refers to the dependence on $\langle X \rangle$ of $f(X)$ written as $f(\bar{X} + \langle X \rangle)$, and so $\partial f(X)/\partial \langle X \rangle = f'(X)$. Then the following identity holds

$$f(X + Z) = \hat{T}_X \sum_k \frac{1}{k!} \langle f^{(k)}(X) \rangle (Z + \bar{X})^k. \tag{28}$$

This is easily proved as follows

$$\begin{aligned}
f(X + Z) &= \sum_n \frac{1}{n!} \langle f^{(n)}(X) \rangle Z_n \\
&= \sum_{n,k} \frac{1}{k!} \beta_{n-k} \langle f^{(n)}(X) \rangle (Z + \bar{X})^k \\
&= \sum_{r,k} \frac{1}{k!} \beta_r \langle f^{(k+r)}(X) \rangle (Z + \bar{X})^k \\
&= \hat{T}_X \sum_k \frac{1}{k!} \langle f^{(k)}(X) \rangle (Z + \bar{X})^k.
\end{aligned} \tag{29}$$

Let us now turn to the application of the previous results to compute the generalized heat kernel expansion. As is well-known the effective action of the complex bosonic field with Klein-Gordon operator Δ is $-\text{Tr}(\log(\Delta))$ (where Tr refers to functional trace). This and related functionals can be obtained once the ‘‘current’’ $\langle x | \Delta^{-1} | x \rangle$ is known.² In the standard case when $M = m^2$ is a c-number the current can be expanded as

²It is understood that the current is known for the whole family of operators $\Delta - \lambda$ for any complex λ , then

$$\text{Tr} f(\Delta) = - \int d^d x \int_{\Gamma} \frac{d\lambda}{2\pi i} f(\lambda) \text{tr} \langle x | \frac{1}{\Delta - \lambda} | x \rangle$$

where the path Γ encloses the spectrum of Δ [4].

$$\langle x|\Delta^{-1}|x\rangle = \sum_{n=0}^{\infty} (-1)^n I_{n+1} a_n, \quad (30)$$

where

$$I_n = \int \frac{d^d p}{(2\pi)^d} \frac{1}{(m^2 + p^2)^n} \quad (31)$$

(d being the spacetime dimension) and a_n are the (diagonal) heat kernel coefficients. They are polynomials of dimension $2n$ constructed with Y , $F_{\mu\nu} = [D_\mu, D_\nu]$ and their covariant derivatives and they do not explicitly depend on d . At lowest orders

$$\begin{aligned} a_0 &= 1, \\ a_1 &= Y, \\ a_2 &= Y^2 - \frac{1}{3}[D_\mu, [D_\mu, Y]] + \frac{1}{6}F_{\mu\nu}F_{\mu\nu}. \end{aligned} \quad (32)$$

(Our convention is that of [12,5] which differs from that of [1] by a factor $(-1)^n/n!$) The lowest order integrals I_n are ultraviolet divergent and so some renormalization is understood. Because the corresponding heat kernel coefficients are polynomials, this renormalization translates into the standard polynomial ambiguity in the effective action (and current etc) in its ultraviolet divergent contributions.

Quite naturally, in the general case of arbitrary M the generalized heat kernel coefficients b_n are defined as [7,8]

$$\langle x|\Delta^{-1}|x\rangle = \sum_{n=0}^{\infty} (-1)^n I_{n+1} b_n, \quad (33)$$

where now

$$I_n = \int \frac{d^d p}{(2\pi)^d} \left\langle \frac{1}{(M + p^2)^n} \right\rangle \quad (34)$$

and the average $\langle \rangle$ refers to flavor space.

Before embarking in the task of computing these generalized coefficients from scratch, it is advisable to rest a moment and consider what result is to be expected. The formulas regarding the expansion of $f(X + Z)$ are fairly general (no assumption was made on the vector space V), but of course they are formal due to ultraviolet divergences when applied to the operator Δ . Technically a very definite problem in these calculations is the lack of cyclic property of the trace when the operator D_μ (or ∂_μ) is involved. In order to avoid these complications, let us temporarily neglect the contributions from derivatives. The simplest way to achieve this is to work in a zero dimensional spacetime, but still with flavor degrees of freedom. In this case Δ equals $U = M + Y$ and this corresponds to $X = M$ and $Z = Y$ in the previous formulas. Expanding the current $(M + Y)^{-1}$ yields $I_n = \langle (m^2)^{-n} \rangle$ and $a_n = Z^n = Y^n$ in the standard expansion (30) and $I_n = \langle M^{-n} \rangle$ and $b_n = Z_n$ in the generalized case (33).

Z_n is given in eq. (24) as a definite combination of Z^n but with Z shifted by \bar{X} . In our case \bar{X} corresponds to

$$\bar{M} = M - \langle M \rangle. \quad (35)$$

Therefore in the present case we obtain a simple relation between standard and generalized heat kernel coefficients, namely

$$b_n = \sum_{k=0}^n \frac{n!}{k!} \beta_{n-k} a'_k \quad (36)$$

where a'_n denotes the usual heat kernel coefficient but using everywhere

$$Y' = Y + \bar{M} \quad (37)$$

instead of Y . In addition, the quantities β_n are given by the same formulas (25,26) with $\bar{x}_n = \langle \bar{M}^n \rangle$.

In fact the same simple relation holds in any number of dimensions for those terms not involving covariant derivatives in a_n and b_n . This is because all these contributions to the current are of the form $f(U)$ (where f depends on the spacetime dimension) and the coefficients are independent of the function f .

Because the simple relation (36) is perfectly well-defined and sensible also in presence of covariant derivatives it can be conjectured that it holds in general. In fact this is the case, as it will be shown subsequently. This is our main result. To lowest orders

$$\begin{aligned} b_0 &= 1, \\ b_1 &= Y + \bar{M}, \\ b_2 &= (Y + \bar{M})^2 - \frac{1}{3}[D_\mu, [D_\mu, Y + \bar{M}]] + \frac{1}{6}F_{\mu\nu}F_{\mu\nu} - \langle \bar{M}^2 \rangle. \end{aligned} \quad (38)$$

The analogous relation holds for the traced and integrated (over x) coefficients needed for the effective action. We have verified that the results in [7] for the traced coefficients b_0, b_1, b_2, b_3, b_4 in $SU(2)$ are reproduced. We remark that the replacement $Y \rightarrow Y' = Y + \bar{M}$ should be done everywhere in a_n (i.e. in terms with derivatives too). The gauge covariance (in Y) is obvious in a'_n since Y' is itself covariant. Another remark is that the formula (22) is not sufficient to obtain the result, in fact it does not even guarantee gauge invariance (in A_μ), and the more detailed formula (24) is needed.

Let us now turn to the proof of the relation (36). The main observation is that we do not really need to compute the generalized coefficients but only to relate them to the standard ones. Therefore our strategy will be to start the computation of the coefficients and at some point recognize that the relation (36) will be obtained.

There is an abundant literature on the computation of the heat kernel coefficients in various settings [5]. Here we will use a method convenient for our present purposes. The first step is to use the method of symbols [13] to express the current

$$\langle x|\Delta^{-1}|x\rangle = \int \frac{d^d p}{(2\pi)^d} \langle x| \frac{1}{(iD_\mu + p_\mu)^2 + U} |0\rangle \quad (39)$$

where $|0\rangle$ is the state with zero momentum $\langle x|0\rangle = 1$, and so $\partial_\mu|0\rangle = 0$. This allows to deal with the ultraviolet divergence $\langle x|x\rangle$ but explicit gauge covariance is lost. Explicit gauge invariance is only recovered after integration over p_μ .

In order to apply our formulas, we identify

$$X = M + p^2, \quad Z = -D^2 + 2ip_\mu D_\mu + Y, \quad (40)$$

regarded as operators in the space of position (spanned by $|x\rangle$) and flavor. p_μ is a c-number parameter. Because X is x -independent the averages $\langle f(X) \rangle$ or $\langle f(\bar{X}) \rangle$ are all in flavor space and well-defined. In particular $\bar{X} = \bar{M}$. Further we define

$$J_n = \left\langle \frac{1}{(M + p^2)^n} \right\rangle, \quad I_n = \int \frac{d^d p}{(2\pi)^d} J_n. \quad (41)$$

A direct application of (10) and (28) then gives

$$\langle x|\Delta^{-1}|x\rangle = \int \frac{d^d p}{(2\pi)^d} \sum_{n=0}^{\infty} (-1)^n J_{n+1} \langle x|Z_n|0\rangle \quad (42)$$

$$= \hat{T}_M \int \frac{d^d p}{(2\pi)^d} \sum_{n=0}^{\infty} (-1)^n J_{n+1} \langle x|(Z + \bar{M})^n|0\rangle. \quad (43)$$

In this formula the operator \hat{T}_M acts on the J_n . It is given in (27) and the β_n are constructed with $\bar{x}_k = \langle \bar{M}^k \rangle$.

A calculation of the coefficients would now proceed as follows: (i) expanding the binomial, (ii) using angular averaging in momentum space, (iii) using integration by parts in momentum space (this step groups together terms with a same dimension where it counts only the dimension carried by D_μ and $Y' = Y + \bar{M}$ but not that carried by the momentum), and (iv) bringing the expression to an explicit form where the operators D_μ appear in covariant derivatives (i.e. in commutators) only. These manipulations produce terms where all operators are purely multiplicative (all derivative operators are already inside commutators) and so equivalent to ordinary functions of x , thus the matrix element $\langle x|0\rangle$ simple evaluates that function at x . This yields the heat kernel coefficients in this approach. (We have explicitly computed b_0 , b_1 and b_2 using this method to verify that no subtleties arise.) However this is not necessary: it can be observed that when M is a c-number \bar{M} vanishes and the formula becomes

$$\langle x|\Delta^{-1}|x\rangle = \int \frac{d^d p}{(2\pi)^d} \sum_{n=0}^{\infty} (-1)^n J_{n+1} (-1)^n \langle x|Z^n|0\rangle. \quad (44)$$

All the manipulations (i-iv) just described can be carried out here and we know that the final result is just the standard heat kernel expansion quoted in (30). Then

when these very manipulations are used in (43) they will produce the same result except that Y is replaced by $Y + \bar{M}$ (the fact that J_n involves an average over flavor does not make any difference). That is,

$$\langle x|\Delta^{-1}|x\rangle = \hat{T}_M \sum_{n=0}^{\infty} (-1)^n I_{n+1} a'_n. \quad (45)$$

Finally, using

$$\frac{\partial I_n}{\partial \langle M \rangle} = -n I_{n+1} \quad (46)$$

produces

$$\langle x|\Delta^{-1}|x\rangle = \sum_{k,n} (-1)^n I_{n+1} \frac{n!}{k!} \beta_{n-k} a'_k \quad (47)$$

and (36) follows.

In summary, developing ideas put forward by Osipov and Hiller, we have presented a general formalism to treat the problem of expanding functionals above non c-number operators while preserving full gauge invariance. We have shown that it is not restricted to formal applications (finite dimensional spaces) since it holds too in presence of ultraviolet divergences. This formalism has been applied to obtain a simple relation (36) between the standard and the generalized heat kernel coefficients introduced in [7,8].

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